

Competition between disorder and Coulomb interaction in a two-dimensional plaquette Hubbard model

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We have studied a disordered $N_c \times N_c$ plaquette Hubbard model on a two-dimensional square lattice at half-filling using a coherent potential approximation (CPA) in combination with a single-site dynamical mean field theory (DMFT) approach with a paramagnetic bath. Such a model conveniently interpolates between the ionic Hubbard model at $N_c = \sqrt{2}$ and the Anderson model at $N_c = \infty$ and enables the analysis of the various limiting properties. We confirmed that within the CPA approach a band insulator behavior appears for non-interacting strongly disordered systems with a small plaquette size $N_c = 4$, while the paramagnetic Anderson insulator with nearly gapless density of states is present for large plaquette sizes $N_c = 48$. When the interaction U is turned on in the strongly fluctuating random potential regions, the electrons on the low energy states push each other into high energy states in DMFT in a paramagnetic bath and correlated metallic states with a quasiparticle peak and Hubbard bands emerge, though a larger critical interaction U is needed to obtain this state from the paramagnetic Anderson insulator ($N_c = 48$) than from the band insulator ($N_c = 4$). Finally, we observe a Mott insulator behavior in the strong interaction U regions for both $N_c = 4$ and $N_c = 48$ independent of the disorder strength. We discuss the application of this model to real materials.

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I. INTRODUCTION

The subtle interplay among kinetic energy, electronic correlation, a periodic ionic potential, and disorder in a two-dimensional electronic system has been an important research topic for several decades and is still under debate^{1,2}. The metal-insulator transition driven by only one energy scale in half-filled two-dimensional systems seems to be relatively well understood: (i) The on-site Coulomb interaction opens a Mott gap, (ii) the periodic ionic potential opens a band gap and (iii) disorder induces an Anderson gap³⁻⁸. However, this is not the case when interactions and disorder compete with electronic itinerancy. There has been a lot of progress on analytical and numerical approaches employed to tackle theoretically the complexity of competing interactions and disorder⁹⁻¹⁷ but a full understanding of this intricate problem is difficult to achieve. Moreover, the existence of a rich variety of real systems where correlation and disorder play an important role such as disordered perovskite compounds, layered dichalcogenide 1T-TaS₂ with Cu intercalation, Sr₂Ir_{1-x}Rh_xO₄ at low doping, nano-arrays on two-dimensional surfaces¹⁸⁻²¹, granular deposits of transition metal-based systems^{22,23}, or two-dimensional metal-oxide-semiconductor field-effect transistors^{24,25} to mention a few, calls for further analysis of this problem.

The ionic Hubbard model with a periodic on-site potential has been intensively studied via various numerical methods such as quantum Monte Carlo and cluster-dynamical mean field theory approaches²⁶⁻³⁰. The re-

sults of these studies differ mostly in details. Overall they describe metallic, bond order, band insulating, antiferromagnetic and paramagnetic (PM) Mott insulating phases. On the other hand, in the absence of Coulomb interactions, the presence of a random disorder that breaks the periodicity of the on-site ionic potential induces a different phenomenon; if the hopping strength of the electrons on a three-dimensional non-interacting system is larger than the fluctuations induced by the random disorder, an Anderson insulator to metal transition appears, while the electrons are always confined in a random potential in one- and two-dimensional non-interacting systems, regardless of the disorder strength⁴. More controversial is, however, the behavior of the disordered system in the presence of Coulomb interactions.

Here we investigate some aspects of this problem by considering a disordered two-dimensional $N_c \times N_c$ plaquette Hubbard model on the square lattice at half-filling. Note that by considering effects of interactions and different plaquette sizes this study goes beyond non-interacting Anderson model and ionic Hubbard model studies. The ionic and Anderson models in the non-interacting limit are recovered for $N_c = \sqrt{2}$ and $N_c = \infty$, respectively. The ionic model with $N_c = \sqrt{2}$ has a gapped density of states $\rho(\omega)$ while $\rho(\omega)$ is gapless and shows a flat behavior around the Fermi level in a coherent potential approximation (CPA) for $N_c = 48$. These features are identified as an Anderson insulator behavior. We have systematically studied in the framework of single-site dynamical mean field theory (DMFT) with a paramagnetic (PM) bath³¹ how $\rho(\omega)$ and the quasiparti-

cle weight Z evolves either from a PM metal, Anderson insulator, or a band insulator to a Mott insulator via tuning of the plaquette size N_c , the Coulomb interaction U and the disorder strength Δ .

We will show that (i) at moderate values of U the system presents a first-order PM metal to Mott insulator transition in the small randomness regime with $\Delta/t = 1$ and 2 for both plaquette sizes $N_c = 4$ and 48, in qualitative agreement with former DMFT results for the system without disorder³². (ii) The non-interacting system with $N_c = 4$ and 48 in the strongly fluctuating potential regions behaves as a band insulator and an Anderson insulator, respectively, and the electrons occupy the low energy states. When interactions are turned on, we find that the electrons lying in low energy states push each other into high energy states and the system becomes a correlated metal with a quasiparticle peak and Hubbard bands in the moderate interaction U region. The critical interaction U_{crit} where the insulator to correlated metal transition occurs is larger in the $N_c = 48$ than in the $N_c = 4$ system. (iii) Finally, in the large interaction region, the systems are Mott insulators independent of disorder strength and plaquette size.

II. MODEL

We consider the following Hamiltonian:

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) - \sum_{i, \sigma} (\mu - \epsilon_i) n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where t describes the electron hopping strength between nearest neighbors, ϵ_i is the on-site energy driven by the random potential at site i , U is the repulsive Coulomb interaction, μ is the chemical potential which is given as $\mu = \frac{U}{2}$ at half-filling, and $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ are the electron creation and annihilation operators at site i with spin σ , respectively. The on-site energies ϵ_i on the $N_c \times N_c$ plaquette sites are sampled randomly from the interval $[-\Delta/t : \Delta/t]$, where Δ is the strength of disorder. The translational invariance of a $N_c \times N_c$ plaquette for a given random disorder is conserved in the system. We set the hopping strength $t = 1$ and the temperature to $T/t = 0.025$ for all single-site dynamical mean field theory (DMFT) calculations with a paramagnetic bath³¹. We employ a continuous-time quantum Monte Carlo algorithm as the DMFT impurity solver^{33,34} in our own implementation³⁵. Disorder effects are evaluated with the coherent potential approximation^{16,36}.

III. RESULTS

A. Non-interacting disordered systems

While a band insulator appears in the non-interacting ionic model limit with $N_c = \sqrt{2}$ at finite Δ/t , an An-

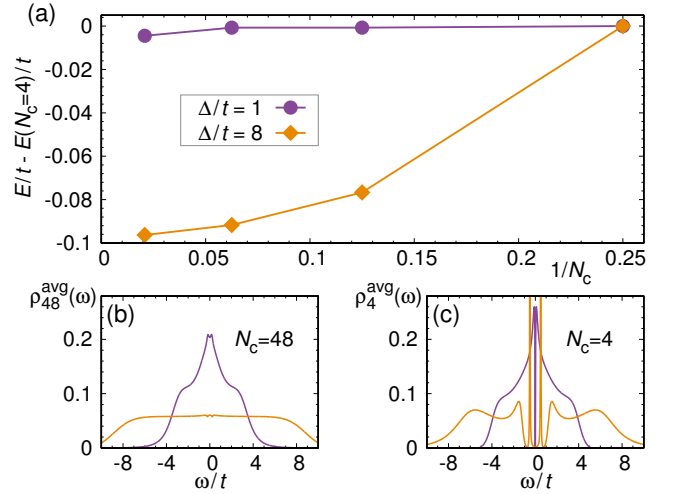


FIG. 1: (Color online) (a) Energies $E/t - E(N_c = 4)/t$ per site as a function of inverse plaquette size N_c^{-1} at $\Delta/t = 1$ and 8 for the non-interacting systems, where $E(N_c = 4)/t$ are the energies per site at $N_c = 4$ for $\Delta/t = 1$ and 8. The values of $E/t - E(N_c = 4)/t$ hardly change with decreasing N_c^{-1} in the weakly disordered regime $\Delta/t = 1$, while they continuously decrease in the strongly disordered regime $\Delta/t = 8$. (b) and (c) show the $\rho_{N_c}^{\text{avg}}(\omega)$ at $N_c = 4$ and 48 for $\Delta/t = 1$ and 8 obtained from the Padé approximation.

derson insulator is observed in a two-dimensional non-interacting disordered system when $N_c = \infty$ at finite Δ/t , according to a standard scaling theory of localization⁴. On the other hand, since we are considering finite $N_c \times N_c$ plaquettes, we estimate that the finite size of the plaquette may disturb a localization of electrons in the two-dimensional non-interacting system with weak disorder whenever the Anderson localization length exceeds the size of plaquette. In order to investigate this behavior, we have studied the non-interacting two-dimensional case both, in the weak and strong disordered regions as a function of plaquette size N_c with the CPA method.

While it has been shown that algebraic averaging one-particle quantities within the CPA approach fail to account for the Anderson localization in the disordered system exactly unlike the recently developed cluster typical medium theory⁸ or typical medium dynamical cluster approximation^{7,16} methods with geometrical average where the density of states $\rho(\omega = 0)$ act as order parameter and disappear at the Fermi level, such a technique is still useful to investigate the trends showed by the system in the different regions of parameter space as we argue below. In the absence of a well defined order parameter in this approximation, a PM Anderson insulator behavior can be identified in terms of a gapless flat density of states near the Fermi level.

We first discuss the energies E of the non-interacting disordered plaquette systems with increasing N_c for several Δ/t obtained from $E = \int d\omega \omega \rho_{N_c}^{\text{avg}}(\omega)$ where $\rho_{N_c}^{\text{avg}}(\omega)$ is the averaged density of states obtained within CPA at N_c . Fig. 1 (a) shows the values of $E/t - E(N_c = 4)/t$

as a function of N_c^{-1} for $\Delta/t = 1$ and $\Delta/t = 8$, where $E(N_c = 4)$ are the energies per site at $N_c = 4$ for $\Delta/t = 1$ and 8. We observe two different behaviors; (i) at small random disorder ($\Delta/t = 1$) $E/t - E(N_c = 4)/t$ remains rather constant as a function of system size N_c , while (ii) at large disorder values $\Delta/t = 8$, the energy continuously decreases with increasing N_c . Our interpretation is that in the case (i), energy states around the Fermi level in a pure system would be only slightly perturbed by impurities and since the Anderson localization length is expected to be much larger than the plaquette size N_c , the energy values are barely changed with increasing N_c . A PM metallic state is then realized where the electrons around the Fermi level are easily pushed into high energy states by small random fluctuations. In this limit of weak disorder the finite plaquette size impedes observing the Anderson insulator expected in the non-interacting case in two dimensions at all disorder strengths. However, for strong random disorder ($\Delta/t = 8$) (case (ii)) the band insulator at small system sizes N_c is manifestly different from the appearance of a PM Anderson insulator at large system sizes.

In order to investigate the differences between cluster sizes $N_c = 48$ and $N_c = 4$ in more detail, we also plot the $\rho_{N_c}^{\text{avg}}(\omega)$ at $N_c = 48$ and 4 for $\Delta/t = 1$ and 8 in Fig. 1 (b) and (c), respectively. At $N_c = 4$, both for $\Delta/t = 1$ and 8 the band insulator is realized. At $N_c = 48$ the slightly perturbed van-Hove singularity at the Fermi level is still present in the weakly fluctuating regime ($\Delta/t = 1$) as it is the case for $\Delta/t = 0$ showing a PM metal behavior, while in the strongly fluctuating regime $\Delta/t = 8$ the van-Hove singularity is completely absent and $\rho^{\text{avg}}(\omega)$ shows a flat behavior around the Fermi level, as expected for a PM Anderson insulator¹³.

B. Interacting disordered systems

We now proceed with the disordered interacting systems with increasing plaquette size N_c . We employ the single-site DMFT approach with temperature $T/t = 0.025$ for these calculations³¹. The DMFT self-consistent equation is given by

$$G_{N_c,\sigma}(i\omega_n) = \int d\epsilon \frac{\rho_{N_c}^{\text{avg}}(\epsilon)}{i\omega_n + \epsilon - \Sigma_{N_c,\sigma}(i\omega_n)}, \quad (2)$$

where ω_n is the Matsubara frequency and the $\rho_{N_c}^{\text{avg}}(\epsilon)$ is the averaged density of states over the cluster of size $N_c \times N_c$ obtained from the CPA approach.

We consider first the weakly fluctuating disordered regime. Fig. 2 (a) and (b) show the quasiparticle weight $Z = (1 - \frac{\text{Im}(\Sigma(i\omega_0))}{\omega_0})^{-1}$ as a function of U/t for systems with two plaquette sizes $N_c = 4$ with ionic potential and $N_c = 48$ with random disorder for $\Delta/t = 1$ and $\Delta/t = 2$, respectively. A first-order PM metal to Mott insulator transition appears in all cases and the coexistence regimes include both PM metal and Mott

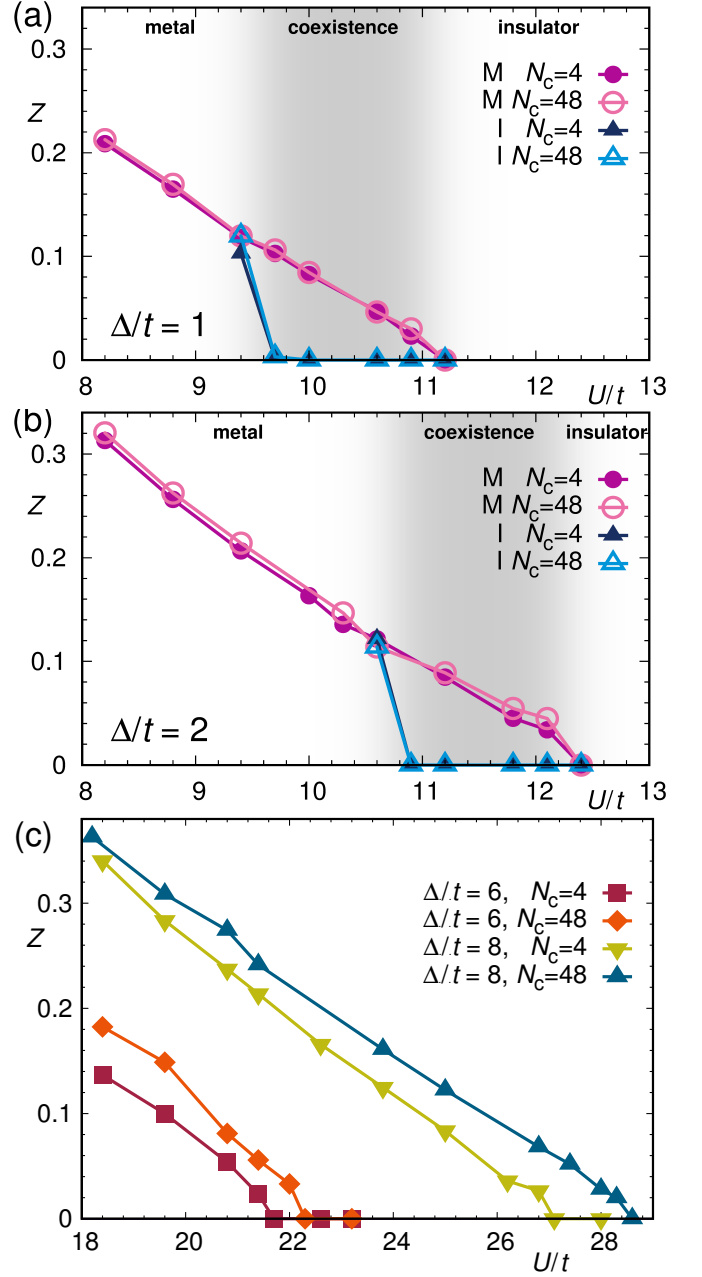


FIG. 2: (Color online) (a) and (b) The quasiparticle weight Z as a function of U/t at $N_c = 4$ and 48 for $\Delta/t = 1$ and 2, respectively. $T/t = 0.025$ for the single-site dynamical mean field theory (DMFT) calculations. "M" and "I" stand for paramagnetic metal and Mott insulator, respectively. First-order PM metal to Mott insulator transitions, where the coexistence regimes including both metal and insulator are clearly seen, are present in all cases with small Δ/t . For both $N_c = 4$ and 48, the critical interactions at $\Delta/t = 1$ are $U_{c1}/t = 9.6$ and $U_{c2}/t = 11.1$; at $\Delta/t = 2$ they are $U_{c1}/t = 10.8$ $U_{c2}/t = 12.3$. The critical interactions U_{c1} and U_{c2} are obtained by starting, respectively, from the insulating and metallic solutions as initial Weiss field. These critical interaction values are comparable to the critical interactions $U_{c1}/t = 9.4$ and $U_{c2}/t = 10.4$ obtained from single-site DMFT calculations in the pure two-dimensional Hubbard model on the square lattice³². (c) The quasiparticle weight Z as a function of U/t at $N_c = 4$ and 48 for $\Delta/t = 6$ and 8. The coexistence regions are not observed in all cases with large Δ/t .

insulator behavior. We also reproduce previous results for the critical interaction $U_{c1}/t = 9.4$ ($U_{c2}/t = 10.4$) of former single-site DMFT on the square lattice for $\Delta/t = 0$ ³². The critical U values increase with disorder strength to $U_{c1}/t = 9.6$ ($U_{c2}/t = 11.1$) for $\Delta/t = 1$ and $U_{c1}/t = 10.8$ ($U_{c2}/t = 12.3$) for $\Delta/t = 2$ and are almost independent of the system size with only tiny differences between the Z values for $N_c = 4$ and $N_c = 48$. These results suggest that if a weak ionic potential (as the case $N_c = 4$) or disorder (as the case $N_c = 48$) are included in a pure DMFT system with moderate Coulomb interaction, any effect driven by the ionic potential or by the random disorder is strongly mitigated by the strong frustration between the averaged local impurity and the PM bath in DMFT. Therefore, even though in a non-interacting system a weak ionic potential ($N_c = 4$) induces a gapped insulator (see Fig. 1) and, random disorder ($N_c = 48$) induces an Anderson insulator, the physics exhibited in all weakly interacting systems with small Δ/t values would be in agreement with the single-site DMFT results of a pure system without random disorder Δ/t . In this weakly interacting and weakly disordered regime, strong frustration effects between impurity sites and paramagnetic bath lead to the metallic state.

Next, we discuss the behavior of the electronic correlated system in the strongly fluctuating disordered regime where a band insulator with a relatively large gap ($N_c = 4$) and a PM Anderson insulator ($N_c = 48$) with a continuous broadened energy band around the Fermi level in the CPA approach are realized in the non-interacting case. We first investigate the behavior of the imaginary part of the self-energy $\text{Im}\Sigma(i\omega_0)$ and the quasiparticle weight Z . Fig. 2 (c) shows Z as a function of U/t for $\Delta/t = 6$ and $\Delta/t = 8$. Z decreases with increasing U/t in all cases. However for $N_c = 48$ the Mott insulator behavior ($Z = 0$) appears at larger U/t values than for $N_c = 4$. Moreover, we have not observed a coexistence regime, unlike the results observed for the first-order PM metal to Mott insulator transition in the weakly random disordered regime in Fig. 2 (a) and (b).

In the following, since $\beta G(\tau = \beta/2)$ is approximately equal to the energy density at the Fermi level ($\beta G(\tau = \beta/2) \approx \rho(\omega = 0)$), we would like to check by computing $\beta G(\tau = \beta/2)$, whether the system shows a gapped or gapless state at the Fermi level ($\omega = 0$). In Fig. 3 $\beta G(\tau = \beta/2)$ is plotted as a function of U/t at $\Delta/t = 8$ for both system sizes $N_c = 4$ and $N_c = 48$. The non-interacting system with $N_c = 4$ at $\Delta/t = 8$ is a band insulator with an energy gap of 1.0 and, as expected, $\beta G(\tau = \beta/2)$ indicates an insulating behavior at $U/t = 0$. The gapped state remains up to $U/t = 12$, where the electrons with up and down spin simultaneously occupy the lowest energy sites. For $U/t > 12$, the electron with spin up (or down) pushes the electron with spin down (or up) at the same site to high energy levels due to the repulsive Coulomb interaction and these ‘pushed up’ electrons are freely moving in the high energy levels. This creates a metallic state in the moderately interacting regions be-

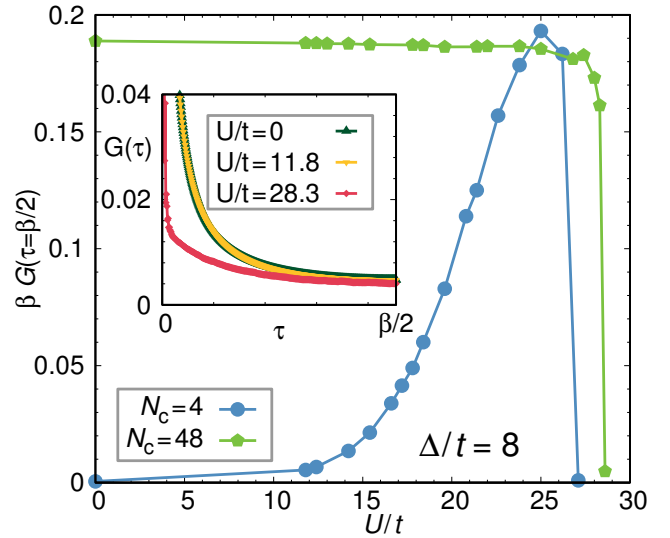


FIG. 3: (Color online) $\beta G(\tau = \beta/2)$ as a function of U/t at $\Delta/t = 8$ and $\beta t = 40$ for $N_c = 4$ and 48 . $\beta G(\tau = \beta/2)$ approximates $\rho(\omega = 0)$, where $\omega = 0$ is the Fermi level. The inset shows $G(\tau)$ for $N_c = 48$ and $\Delta/t = 8$ at three different interaction values $U/t = 0, 11.8$ and 28.3 .

tween $U/t = 14$ and 27 by competition and cooperation of Δ/t and U/t . For large $U/t > 27$, the system becomes a Mott insulator and $\beta G(\tau = \beta/2)$ converges to zero.

The case of $N_c = 48$ is distinctly different. At the value $\Delta/t = 8$ a PM Anderson insulator may be expected for the non-interacting system. As U/t increases, the value $\beta G(\tau = \beta/2) = 0.187$ remains unchanged up to $U/t = 25$. This behavior suggests that the physical state corresponding to a PM Anderson insulator remains up to this U/t value. In the inset of Fig. 3 we have plotted $G(\tau)$ for $U/t = 0, 11.8$, and 28.3 in order to confirm this suspicion. We confirm that $G(\tau)$ for $U/t = 0$ and 11.8 fall on top of each other. This may indicate that for strong disorder the PM Anderson insulator is still preserved in the weakly interacting regime, even though interactions are involved. Around $U/t = 28.3$, $\beta G(\tau = \beta/2)$ shows a kink that hints to the presence of a correlated metallic state due to the fact that interactions push up the electrons of low states into high states. In the strongly correlated regime $U/t > 28.3$ in Fig. 3, $\beta G(\tau = \beta/2)$ converges to zero which indicates the Anderson-Mott insulator behavior.

In order to establish more clearly the various physical phases, we explore $\rho(\omega)$ calculated by a stochastic analytical continuation from $G(i\omega_n)$ ³⁷. Fig. 4 (a) and (b) show $\rho(\omega)$ at $\Delta/t = 8$ and various U/t for $N_c = 4$ and $N_c = 48$, respectively. $\rho(\omega)$ for $N_c = 4$ (Fig. 4 (a)) exhibits a band insulator at $U/t = 11.8$ and a Fermi liquid behavior with a quasiparticle peak at $U/t = 26.8$ and agrees with the results of the density of states at the Fermi level estimate $\beta G(\tau = \beta/2)$ in Fig. 3. $\rho(\omega)$ for $N_c = 48$ (Fig. 4 (b)) shows flat behavior around the Fermi level at $U/t = 11.8$ and this result is similar to that at

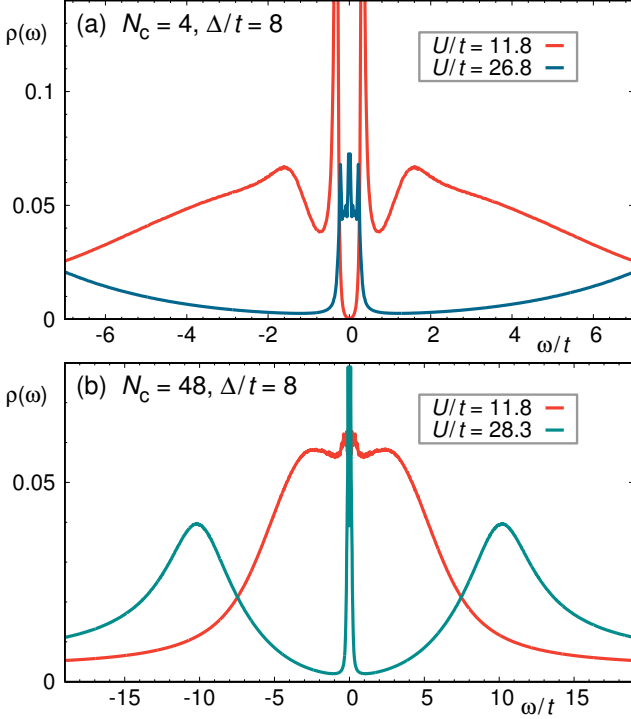


FIG. 4: (Color online) (a) and (b) present the density of states $\rho(\omega)$ of systems with $\Delta/t = 8$, $U/t = 11.8$ and 26.8 for $N_c = 4$ and $U/t = 11.8$ and 28.3 for $N_c = 48$ under the condition of $\rho(\omega) = \rho(-\omega)$ by the particle-hole symmetry, respectively.

$U/t = 0$ (Fig. 1 (b)) which hints to a PM Anderson insulator. At $U/t = 28.3$, $\rho(\omega)$ shows a quasiparticle peak at the Fermi level and a Hubbard band around $\pm\omega/t = 11$. The repulsive Coulomb interaction pushes the electrons at low energies into high energy states inducing an Anderson insulator to correlated metal transition. This region is however very narrow.

IV. CONCLUSIONS

We summarize the results of this study by plotting the phase diagrams for disordered interacting systems at $N_c = 4$ and 48 in Fig. 5 (a) and (b), respectively. Even though the single-site DMFT approach emphasizes local fluctuations in a fully frustrated PM bath and thus overestimates the PM metal regions in both cases, it still captures basic properties of the systems considered such as band insulator, Anderson insulator, correlated metal, and Mott insulator induced by random disorder and electronic correlations. In more detail, the metal to Mott insulator transition in the weak disordered regions are closer to those of DMFT results without disorder because the strong local fluctuations of the DMFT approximation, most probably, overwhelm effects driven by disorder, while we find sandwiched *correlated metallic states* between a band insulator and a Mott insula-

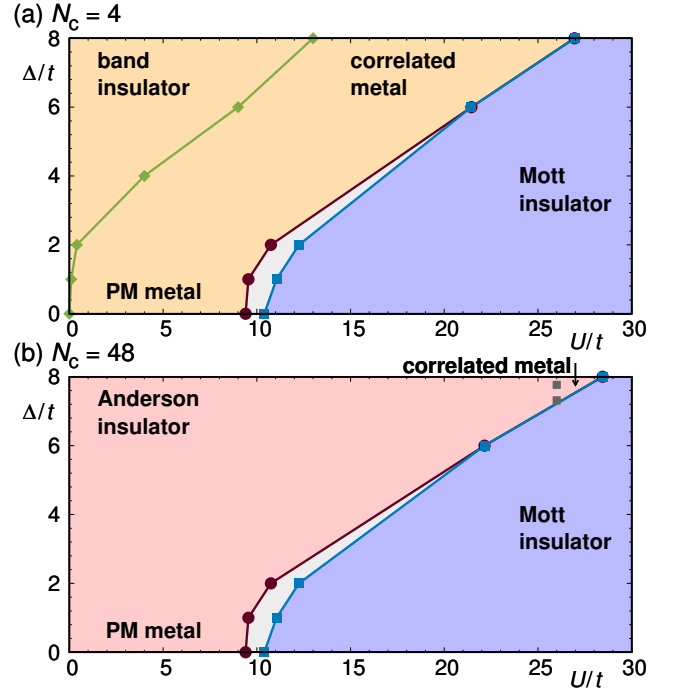


FIG. 5: (Color online) Phase diagrams of the two-dimensional $N_c \times N_c$ plaquette disordered interacting systems at (a) $N_c = 4$ and (b) 48 via the single-site dynamical mean field theory. The coexistence regions including behaviors of both PM metal and Mott insulator are located between the PM metal and the Mott insulator in the weakly disordered regions. The critical interaction U_c is obtained by sweeping in steps of 0.4 the value of the interaction U . The critical interactions U_c at $\Delta/t = 0$ are obtained from Ref. 32. The error bars are given by the size of the symbols. Note that the determination of the crossover line between PM metal and Anderson insulator for the case of $N_c = 48$ in (b) is much more difficult since the physical quantities that account for an accurate phase boundary between Anderson insulator and PM metal are absent within CPA. Therefore, we determine the correlated metallic regimes, where the electrons in low energy states push each other into high energy states, and phase boundary only in the strong disorder region with $\Delta/t = 8$ and $N_c = 48$ in (b), via estimation of $\beta G(\tau = \beta/2)$ of Fig. 3.

tor with $N_c = 4$ and between an Anderson insulator and a Mott insulator with $N_c = 48$ at strong disordered regimes. Such states can be understood by the fact that electrons in the low energy states push each other into high energy states and correlated metallic states with a quasiparticle peak and Hubbard bands emerge.

Even though we considered a simple model, the emergence of the various competing phases as a function of cluster size, electron-electron interaction and disorder may provide further hints, for instance, to the microscopic origin of the metal-insulator transition observed in two-dimensional metal-oxide-semiconductor field-effect transistors^{24,25}. Furthermore, confinement of Fermionic atoms in an optical lattice to realize ionic-type Hubbard models is conceivable and could be guided by our results

for small N_c .

Finally, in view of the physics uncovered in this work for the two-dimensional plaquette Hubbard model, a next step would be, when very fast multi-site impurity solvers become available, to employ the more advanced recently developed typical medium dynamical cluster approximation^{7,8} which can account for nonlocal spatial correlations and for the Anderson localization length beyond the CPA in combination with the DMFT approach.

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